

Exact Topological Twistons in Crystalline Polyethylene

E. Ventura and A. M. Simas

Departamento de Química Fundamental, Universidade Federal de Pernambuco
50670-901, Recife, Pernambuco, Brazil

and

D. Bazeia[†]

Departamento de Física, Universidade Federal da Paraíba
Caixa Postal 5008, 58051-970, João Pessoa, Paraíba, Brazil

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Abstract

We investigate the presence of topological twistons in crystalline polyethylene. We describe crystalline polyethylene with a model that couples the torsional and longitudinal degrees of freedom of the polymeric chain by means of a system of two real scalar fields. This model supports topological twistons, which are described by exact and stable topological solutions that appear when the interaction between torsional and longitudinal fields is polynomial, containing up to the sixth power in the fields. We calculate the energy of the topological twiston, and the result is in very good agreement with the value obtained via molecular simulation.

[†]Corresponding author. Fax: +55 83 216 7542; E-mail: bazeia@fisica.ufpb.br

The existence of twistons in crystalline polyethylene (PE) was postulated [1] two decades ago, and refers to a twist of 180° that extends smoothly over several CH_2 groups in crystalline PE, in the plane orthogonal to the chain direction, with the corresponding CH_2 unit length contraction along the polymeric chain. These twiston configurations appear in crystalline PE as a result of its large torsional flexibility, and may contribute to elucidate some of its properties, in particular the dielectric α relaxation [2, 3, 4, 5, 6, 7].

There are some interesting models of twistons in crystalline PE [8, 9, 10, 11, 12]. The works [8, 9] are almost simultaneous to the work [13], which introduces solitons to describe conductivity in polyacetylene via distortions of the single-double bond alternations. In the PE chain, however, the bounds are always single bounds, which require at least one bosonic degrees of freedom to describe the torsional flexibility of this unsaturated polymer. Despite these two decades of investigations, we believe that the issue of topological twistons playing some role in explaining properties of the crystalline PE chain is still incomplete, requiring further investigations both in the theoretical and experimental grounds. This is the main motivation of the present work, where we follow an alternate route to topological twistons in PE to bring new facts to the former theoretical investigations. This new route was introduced in Ref. [14], and here we complete the investigation, including the calculation of the energies of the exact topological twistons.

We start our investigations by first reviewing the basic features of the several distinct mechanical models used to describe twistons in crystalline PE. The most important ones are described in Refs. [8, 9, 10, 11, 12]. In the pioneer work [8] the author considers a system which couples the torsional and translational degrees of freedom. In Ref. [9] the authors consider a simpler system, describing only the torsional motion along the crystalline chain, and this is also considered in the subsequent work [10]. It is only more recently [11, 12] that one includes interactions between radial, torsional and longitudinal degrees of freedom. In this case one uses cylindrical coordinates to describe a generic CH_2 unit via (r_n, θ_n, z_n) , which correspond to the three degrees of freedom of the rigid molecular group. A simplification can be introduced, and concerns freezing the r_n 's, so that the radial motion is neglected. In [11] one further ignores the translational degree of freedom, the z_n coordinates, to get to a simple model described via the torsional variable that in the continuum limit can be taken as $\theta_n(t) \rightarrow \theta(z, t)$. The model reproduces the double sine-Gordon model, according to the assumptions there considered to describe the intermolecular interaction. The other more recent work [12] on twiston in crystalline PE gives another step toward a more realistic model. This is the first time the radial, torsional and longitudinal degrees of freedom are simultaneously considered to model twiston in crystalline PE. The model is very interesting, although it is hard to find exact solutions and investigate the corresponding issues of stability. The problem engenders several intrinsic difficulties, which have inspired us to search for an alternate model, in the form of two coupled fields belonging to the class of systems investigated in the recent works [15, 16, 17, 18].

The basic assumptions introduced in the former models for twistons in crystalline PE may be described considering cylindrical coordinates. The Lagrangian presents the usual form $L = T - U$,

where

$$T = \frac{1}{2} m \sum_n (\dot{r}_n^2 + r_n^2 \dot{\theta}_n^2 + \dot{z}_n^2) \quad (1)$$

$$U = U_{\text{intra}} + U_{\text{inter}} \quad (2)$$

Here m is the mass associated to the molecular group CH_2 , and U_{intra} and U_{inter} are potentials used to model the intramolecular and intermolecular interactions in the crystalline environment, respectively. The intramolecular potential can be considered as

$$U_{\text{intra}} = \frac{1}{2} \sum_n K_1 (\theta_{n+1} - \theta_n)^2 + \frac{1}{2} \sum_n K_2 (z_{n+1} - z_n)^2 + \dots \quad (3)$$

where K_1 and K_2 are coefficients related to the harmonic approximation for torsional and longitudinal motions, respectively. The intramolecular potential may contain derivative coupling between the torsional and longitudinal motions. In this case we should add to U_{intra} the contribution [11]

$$\frac{1}{2} \sum_n K_3 (\theta_{n+1} - \theta_n)^2 (z_{n+1} - z_n) \quad (4)$$

However, instead of the above coupling we can consider derivative coupling between the radial and longitudinal motions. In this other situation we add to U_{intra} the contribution [12]

$$\frac{1}{2} \sum_n K_4 (r_n - r_0)^2 + \frac{1}{2} \sum_n K_5 (r_{n+1} - r_n) (z_{n+1} - z_n) \quad (5)$$

The above terms (4) and (5) are two among several other possibilities of introducing derivative coupling between the torsional, longitudinal and radial degrees of freedom. We shall not consider such possibilities in the present work, although in [18] one shows a route for taking derivative coupling into account. As we are going to show below, we consider the standard harmonic approximation for U_{intra} in order to follow the basic steps of the first works [8, 9, 10] on twistons in crystalline PE.

The second potential in (2) is U_{inter} . It responds for the intermolecular interactions and is usually given in the form $U_{\text{inter}} = \sum_n [U_0(\theta_n) + U_1(\theta_n) U_l(z_n)]$. Here $U_0(\theta_n)$ and $U_1(\theta_n)$ are used to model torsional mobility and $U_l(z_n)$ to describe the longitudinal motion along the chain. In the works [8, 9, 10, 11], after freezing radial and translational motion, the above intermolecular potential is described by the $U_0(\theta_n)$ contributions. We can get to models for the torsional motion alone, and in the continuum limit they may be described via the sine-Gordon potential [8, 9, 10] $A_1 [1 - \cos(2\theta)]$, or the polynomial potential [9] $A_2 \theta^2 + B_1 \theta^4$, or yet the double sine-Gordon potential [11] $A_3 [1 - \cos(2\theta)] + B_2 [1 - \cos(4\theta)]$. Here A_i and B_i are real constants, used to parametrize the corresponding interactions. Evidently, the above potentials lead to different models for the torsional field, and are introduced to account for the specific motivations presented in the respective works [8, 9, 10, 11]. In the more recent work [12], one considers coupling

between the radial, torsional and longitudinal degrees of freedom, but the analytical solutions there obtained are found under assumptions that ultimately decouple the system.

The above models show that the basic idea introduced in Ref. [1] has survived along the years, although there have been interesting quantitative contributions to investigate the presence of twistons in crystalline PE. In particular, in Ref. [12] one includes the most relevant degrees of freedom when one considers the CH_2 group in the form of rigid molecular group along the crystalline chain in crystalline PE. However, in the model considered in [12] we could not fully understand the reason for not considering harmonic interactions between neighbor radial coordinates, while taking into account interactions between radial and longitudinal degrees of freedom in the intramolecular potential. For this reason, we think we can introduce another mechanical model for the polymeric chain, where we modify some assumptions presented in the former works [11, 12]. The difficulties inherent to the problem of describing topological twistons in crystalline PE bring motivations for simplifying former assumptions, with the aim of offering an alternate model that presents exact solutions for twistons in crystalline PE. Toward this goal, let us use cylindrical coordinates to describe the molecular groups under the assumption of rigidity. We start with the kinetic energy (1), rewriting it in the form

$$T = \frac{1}{2} m r_0^2 \sum_n \left(\dot{\phi}_n^2 + \left(\frac{c}{r_0} \right)^2 \dot{\chi}_n^2 + \dot{\rho}_n^2 \right) \quad (6)$$

Here we have set $\phi_n = \theta_n - [1 - (-1)^n](\pi/2)$, $\chi_n = (z_n - nc)/c$ and $\rho_n = (r_n - r_0)/r_0$, where r_0 is the equilibrium position of the radial coordinate and c is the longitudinal distance between consecutive molecular groups. Now ϕ_n , χ_n and ρ_n are all dimensionless variables, and in the continuum limit they can be seen as real fields $\phi(z, t)$, $\chi(z, t)$ and $\rho(z, t)$. Before going to the continuum version of the PE chain, however, let us reconsider the intramolecular potential given by Eq. (3). We use the harmonic approximation to write

$$U_{\text{intra}} = \frac{1}{2} \sum_n k_t (\phi_{n+1} - \phi_n)^2 + \frac{1}{2} \sum_n k_l (\chi_{n+1} - \chi_n)^2 + \frac{1}{2} \sum_n k_r (\rho_{n+1} - \rho_n)^2 \quad (7)$$

where k_t , k_l and k_r are spring-like constants, related to the torsional, longitudinal and radial degrees of freedom, respectively.

The harmonic interactions present in the intramolecular term (7) makes the dynamics to appear as the dynamics of relativistic fields, in the same way it happens with the standard harmonic chain. We use (6) and (7) to write the following Lagrangian density for the continuum version of the mechanical model for crystalline PE

$$\begin{aligned} \mathcal{L}_m = & \frac{1}{2} \frac{m}{c} r_0^2 \left(\frac{\partial \phi}{\partial t} \right)^2 - \frac{1}{2} k_t c \left(\frac{\partial \phi}{\partial z} \right)^2 + \frac{1}{2} \frac{m}{c} c^2 \left(\frac{\partial \chi}{\partial t} \right)^2 - \\ & \frac{1}{2} k_l c \left(\frac{\partial \chi}{\partial z} \right)^2 + \frac{1}{2} \frac{m}{c} r_0^2 \left(\frac{\partial \rho}{\partial t} \right)^2 - \frac{1}{2} k_r c \left(\frac{\partial \rho}{\partial z} \right)^2 - V_{\text{inter}}(\phi, \chi, \rho) \end{aligned} \quad (8)$$

The quantity m/c identifies the mass density along the chain, and $k_t c = \kappa_t$, $k_l c = \kappa_l$, $k_r c = \kappa_r$ are Young parameters related to the torsional, longitudinal and radial motion, respectively.

The above mechanical model is still incomplete, but it contains the basic assumption that we are dealing with an harmonic chain, and deviation from the harmonic behavior is to be included in V_{inter} . Although in this case we can not introduce any other derivative coupling, we still have the freedom to specify V_{inter} and so introduce nonlinearity via the presence of the surrounding environment in the crystalline material. This is the model we keep in mind to introduce the following field theoretic considerations.

We follow the lines of the former mechanical model, which lead us to introduce a field theoretic model that contains three real scalar fields. The Lagrangian density describing the fields $\phi = \phi(x, t)$, $\chi = \chi(x, t)$ and $\rho = \rho(x, t)$ was introduced in Ref. [14]. The model is defined by the potential, which is supposed to have the form

$$V(\phi, \chi, \rho) = \frac{1}{2}H_\phi^2 + \frac{1}{2}H_\chi^2 + \frac{1}{2}H_\rho^2 \quad (9)$$

Here $H_\phi = \partial H / \partial \phi$ and so forth. $H = H(\phi, \chi, \rho)$ is a smooth but otherwise arbitrary function of the fields. This restriction is introduced along the lines of the former investigations [15, 16, 17], and leads to interesting properties, such as the ones explored below.

We focus attention on the crystalline PE chain. In this case it is a good approximation [8, 9, 10, 11, 12] to discard radial motion in the PE chain. This simplification leads to a system of two fields, describing torsional and longitudinal motions simultaneously. However, we first consider the simpler system, described by the torsional field alone. In this case, in accordance with the Refs. [11, 12], investigations on molecular simulation allows introducing the following torsional potential

$$V_1(\phi) = \frac{1}{2}\lambda^2\phi^2(\phi^2 - \pi^2)^2 \quad (10)$$

Fortunately, this potential is generated by the function $H_1(\phi) = (1/2)\lambda\phi^2(\phi^2/2 - \pi^2)$. Also, it has three degenerate minima, one at $\phi = 0$ and the other two at $\phi^2 = \pi^2$.

We use the potential $V_1(\phi)$ to get the masses of the elementary excitations around $\phi = 0$ and $\phi = \pm\pi$ in the form $m_\phi(0) = |\lambda|\pi^2$ and $m_\phi(\pm\pi) = 2|\lambda|\pi^2$. These results identify an asymmetry in the spectra of excitations of the torsional motion around the minima $\phi = 0$ and $\phi^2 = \pi^2$. This asymmetry appears in consequence of the polynomial potential (10), and is small for small λ . It is related to the asymmetry between the well at $\phi = 0$, and the well at $\phi^2 = \pi^2$. Since the mass of the field corresponds to the minimum energy necessary to excite elementary mesons into the system, we realize that the value $|\lambda|\pi^2$, the difference $2|\lambda|\pi^2 - |\lambda|\pi^2$ may be seen as the energy for the field ϕ go from $\phi = 0$ to $\phi = \pm\pi$, that is the energy to overcome the torsional barrier in this simplified model.

To get to a more realistic model we couple the torsional field to the longitudinal motion along the chain. We model the presence of interactions by extending the former function $H_1(\phi)$ to $H_2(\phi, \chi)$ given by

$$H_2(\phi, \chi) = \frac{1}{2}\lambda\phi^2\left(\frac{1}{2}\phi^2 - \pi^2\right) + \frac{1}{2}\mu\phi^2\chi^2 \quad (11)$$

This gives the system

$$\mathcal{L}_2 = \frac{1}{2} \left(\frac{\partial \phi}{\partial t} \right)^2 - \frac{1}{2} \left(\frac{\partial \phi}{\partial z} \right)^2 + \frac{1}{2} \left(\frac{\partial \chi}{\partial t} \right)^2 - \frac{1}{2} \left(\frac{\partial \chi}{\partial z} \right)^2 - V_2(\phi, \chi) \quad (12)$$

where

$$V_2(\phi, \chi) = \frac{1}{2} \lambda^2 \phi^2 (\phi^2 - \pi^2)^2 + \lambda \mu \phi^2 (\phi^2 - \pi^2) \chi^2 + \frac{1}{2} \mu^2 \phi^2 \chi^4 + \frac{1}{2} \mu^2 \phi^4 \chi^2 \quad (13)$$

We are using natural units, as in Ref. [14]. The above potential presents interesting features. For instance, $V_2(\phi, 0) = V_1(\phi)$, which reproduces the torsional model $V_1(\phi)$ when one freezes the longitudinal motion. Also, $V_2(0, \chi) = 0$ and

$$V_2(\pm\pi, \chi) = \frac{1}{2} \mu^2 \pi^4 \chi^2 + \frac{1}{2} \mu^2 \pi^2 \chi^4 \quad (14)$$

We can evaluate the quantity $\partial^2 V / \partial \phi \partial \chi$ to see that it contributes with vanishing values at the minima $(0, 0)$ and $(\pm\pi, 0)$. This shows that the spectra of excitations of the torsional motion around the ground states are unaffected by the presence of the longitudinal motion. Thus, we can use $V_1(\phi)$ to investigate the behavior of the torsional motion around the equilibrium configurations.

The masses of the ϕ field are now given by $m_\phi(0, 0) = |\lambda|\pi^2$ and $m_\phi(\pm\pi, 0) = 2|\lambda|\pi^2$, around the minima $(0, 0)$ and $(\pm\pi, 0)$, respectively. Accordingly, for the χ field we see that it is massless at $(\phi = 0, \chi = 0)$, and at $(\pm\pi, 0)$ the mass is $m_\chi(\pm\pi, 0) = |\mu|\pi^2$. These results identify an asymmetry in the spectra of excitations of both the torsional and longitudinal motion around the minima $(0, 0)$ and $(\pi^2, 0)$. This asymmetry appears in consequence of the polynomial potential (13), and is small for small parameters λ and μ . These results allow introducing the ratio m_χ/m_ϕ between the masses of the ϕ and χ fields – see Ref. [14].

The topological solutions connect distinct, adjacent minima of the potential. The energy corresponding to the classical configurations can be written in the general form [17]

$$E_{ij} = |H(\bar{\phi}_i, \bar{\chi}_i, \bar{\rho}_i) - H(\bar{\phi}_j, \bar{\chi}_j, \bar{\rho}_j)| \quad (15)$$

where $(\bar{\phi}_i, \bar{\chi}_i, \bar{\rho}_i)$ and $(\bar{\phi}_j, \bar{\chi}_j, \bar{\rho}_j)$ stand for two vacuum states, that is, two adjacent points i and j in the field space (ϕ, χ, ρ) that minimize the potential.

Let us first consider the case of a single field, the ϕ field that describes torsional motion along the polymeric chain. We use former results to write the equation of motion for static configuration in the form

$$\frac{d^2 \phi}{dz^2} = \lambda^2 \phi (\phi^2 - \pi^2) (3\phi^2 - \pi^2) \quad (16)$$

This equation is solved by solutions of the first-order equation

$$\frac{d\phi}{dz} = \lambda \phi (\phi^2 - \pi^2) \quad (17)$$

There are topological twistons, given by [15]

$$\phi_{(t)}^{(\pm)}(z) = \pm \pi \sqrt{(1/2)[1 - \tanh(\lambda\pi^2 z)]} \quad (18)$$

Here we are taking $z = 0$ as the center of the soliton, but this is unimportant because the continuum, infinity chain presents translational invariance. The sign of λ identifies kink and antikink solutions, connecting the minima 0 and π or 0 and $-\pi$. These solutions are stable and can be boosted to their time-dependent form by just changing z to $\xi = (z - vt)/(1 - v^2)^{1/2}$. This model can be seen as an alternate model to the ones introduced in the former works [8, 9, 10, 11].

The amplitude of the torsional field ϕ is π , which is the angle the chain rotates to form the twiston. The width of the twiston, $L_{(t)}$, which is the length along the chain where the angular position of CH_2 groups appreciably deviates from the crystallographic positions, is inversely proportional to the quantity $|\lambda|\pi^2$. We can also get the energy corresponding to the static twiston. We use Eq. (15) to get the value

$$E_{(t)} = \frac{1}{4}|\lambda|\pi^4 \quad (19)$$

We now consider the model that describes interactions between the torsional and longitudinal fields. The equations of motion for static fields $\phi = \phi(z)$ and $\chi = \chi(z)$ are given by

$$\frac{d^2\phi}{dz^2} = \lambda^2\phi(\phi^2 - \pi^2)(3\phi^2 - \pi^2) + 2\lambda\mu\phi(2\phi^2 - \pi^2)\chi^2 + \mu^2\phi(\chi^2 + 1)\chi^2 \quad (20)$$

$$\frac{d^2\chi}{dz^2} = 2\lambda\mu\phi^2(\phi^2 - \pi^2)\chi + 2\mu^2\phi^2\chi^3 + \mu^2\phi^2\chi \quad (21)$$

Although there is no general way of solving these equations, we recognize that they follow from the potential in Eq. (13), defined via the function introduced in Eq. (11), and so they are solved by

$$\frac{d\phi}{dz} = \lambda\phi(\phi^2 - \pi^2) + \mu\phi\chi^2 \quad (22)$$

$$\frac{d\chi}{dz} = \mu\phi^2\chi \quad (23)$$

which are first-order differential equations, easier to investigate.

To find explicit solutions we use the trial orbit method introduced in Ref. [19]. We consider the orbit

$$\lambda(\phi^2 - \pi^2) + \mu\chi^2 = \mu(\phi^2 - \pi^2) \quad (24)$$

We note that this orbit is compatible with the first-order Eqs. (22) and (23). Also, from Eq. (22) we get

$$\phi_{(t,l)}^{(\pm)}(z) = \pm \pi \sqrt{(1/2)[1 - \tanh(\mu\pi^2 z)]} \quad (25)$$

This result and the orbit (24) are now used to obtain,

$$\chi_{(t,l)}^{(\pm)}(z) = \pm \pi \sqrt{\frac{\lambda}{\mu} - 1} \sqrt{(1/2)[1 + \tanh(\mu\pi^2 z)]} \quad (26)$$

These solutions are valid for $\lambda/\mu > 1$ and are similar to the solutions found in Ref. [12] to describe the torsional and longitudinal degrees of freedom that describe topological twistons in the crystalline PE chain.

The amplitude of the twiston is still π , while the amplitude of the longitudinal motion is given by $\pi [(\lambda/\mu) - 1]^{1/2}$. This result requires that $\lambda/\mu > 1$, which is compatible with the investigation of Ref. [14]. In this more sophisticated model the width $L_{(t,l)}$ of the topological twiston is proportional to $1/(|\mu|\pi^2)$. It depends inversely on μ . We compare $L_{(t)}$ and $L_{(t,l)}$ to see that $L_{(t,l)} > L_{(t)}$ since $\lambda/\mu > 1$ for the topological twiston of the model of two coupled fields. This result is new, and shows that the presence of the longitudinal motions contributes to enlarge the width of the topological twiston.

Another result follows after calculating the energy of these solutions. We use Eq. (15) to get $E_{(t,l)} = E_{(t)} = (1/4)|\lambda|\pi^4$, which equals the value of the energy of the simpler model, where one discards the motion of the longitudinal field. This result shows that although the more general model changes some of the features of the simpler model, which describes only the twiston field, it does not change the energy of the twiston. We understand this result as follows: the first-order equations (22) and (23) also present the pair of solutions

$$\bar{\phi}_{(t,l)}^{(\pm)}(z) = \pm \pi \sqrt{(1/2)[1 - \tanh(\lambda\pi^2 z)]} \quad \bar{\chi}_{(t,l)}(z) = 0 \quad (27)$$

This pair of solutions and the former one, given by Eqs. (25) and (26), are at the same topological sector and present the very same energy, given in Eq. (??). However, when one sets $\chi \rightarrow 0$ in the coupled model, the system changes to the simpler model, and so the energy of the pair (27) is necessarily equal to the energy of the twiston in the single field system. This fact explains our results, and shows that the torsional energy is the main quantity to calculate the energy of the topological twiston. We use this point of view to rewrite the energy as $E_{(t,l)} = (1/4)(|\lambda|\pi^2)\pi^2$. We have already identified $|\lambda|\pi^2$ and $2|\lambda|\pi^2$ as the masses of the twiston field, which show that when the ϕ field varies from 0 to $\pm\pi$, that is when a twiston is formed, one changes from the energy $|\lambda|\pi^2$ to the energy $2|\lambda|\pi^2$, and this requires the value $|\lambda|\pi^2$. We then identify this value with the energy for twiston formation along the polymeric chain. According to Ref. [1], the energy contribution of the localized twisted region to the creation of the twist defect is 7.3 Kcal/mol. In fact, in Fig. [6] and Table II of Ref. [1] we see that $U_0 = 9.8 - 2.5 = 7.3$ Kcal/mol, which is to be regarded as the contribution of the localized twisted region to the creation of the twist defect [20]. We then change $|\lambda|\pi^2 \rightarrow 7.3$ in the energy to obtain

$$E_{(t,l)} = 17.99 \text{ Kcal/mol} \quad (28)$$

This is the energy of the topological twiston, and is in good agreement with the energy values of 18.01 Kcal/mol [1], 18-19 Kcal/mol [10], and 17.2 Kcal/mol [12], obtained using different numerical simulations and models.

We conclude this letter recalling that we have investigated a system of two coupled real scalar fields to model topological twistons in crystalline PE. This model describes no radial motion, but it couples the torsional and longitudinal degrees of freedom in a very interesting way. We have found exact solutions, which engender several features, and here we offer the following remarks. The limit $\mu \rightarrow \lambda$ transforms the solutions (25) and (26) into the solutions (18) of the former case, that describes the torsional motion alone. The solutions of the model of a single field present width proportional to $1/|\lambda|$, and for the two field model it is proportional to $1/|\mu|$. The width of the solutions of the two fields is exactly the same, in agreement with the topological features of the solutions, and with the orbit (24), used to solve the coupled equations (22) and (23). This result is intuitive, since one expects that when the torsional motion completes the 180° rotation and returns to its crystallographic position the longitudinal motion should simultaneously return to its crystal register. The amplitude of the torsional field is given by the solution (25) and is π , in agreement with the model we use for the twiston configuration. The amplitude of the longitudinal motion is given by the solution (26) and is $\pi [(\lambda/\mu) - 1]^{1/2}$. In the PE chain we have to set this to unit, to make it compatible with c , the full longitudinal motion. This picture follows in accordance with the fact that crystalline PE presents degenerate ground states, obtained from each other by a rotation of 180° or by a translation of c along the polymer chain.

We have also obtained the energy of the twistons. It is $E = (1/4) |\lambda| \pi^4$. We have used $|\lambda| \pi^2$ to identify the mass difference for the torsional field in the minima $\phi = \pi$ and $\phi = 0$. This and results of Ref. [1] allow getting $|\lambda| \pi^2 = 7.3$ Kcal/mol, which gives the energy of the topological twiston as 17.99 Kcal/mol, in good agreement with values known in the literature.

The results presented in this work completes the former investigation [14]. They show that the approach of using systems of coupled fields and the corresponding field theoretic analysis to describe topologically non-trivial excitations in continuum versions of polymeric chains seems to work correctly. The procedure describes interesting aspects of the problem, and allows obtaining the energy of the topological excitation in a direct way. We believe that similar polymeric chains can also be investigated by similar systems, and this makes us to think on modelling topological twistons for instance in the family of systems where one changes some CH_2 groups by oxygens periodically, to make chains with the basic units CH_2-O , CH_2-CH_2-O , $CH_2-CH_2-CH_2-O$, etc. Despite the presence of oxygen the bounds are still sigma bounds, and the torsional motion seems to be similar to the PE chain. Thus, we may use a twiston model to explore properties of the family $(CH_2)_n - O$, in particular in the case of $CH_2 - CH_2 - O$, the Poly(oxyethylene), POE. This and other related investigations are presently under consideration.

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